M121

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Air Quality Monitoring

Shell Chemicals
Scotford Complex

March 14, 2005 Special Report – Emergency Response

Summary

Alberta Environment conducts mobile air quality surveys each year as part of its air quality monitoring program. These monitoring surveys are unannounced and use the Department's *Mobile Air Monitoring Laboratory* (MAML). The MAML monitoring provides a "snapshot" in time and space of the air quality at the location monitored. Pollutants measured by the MAML included ammonia, carbon monoxide, hydrocarbons (methane, total, reactive and polycyclic aromatic), oxides of nitrogen (NO_2, NO and NO_x), ozone, particulate matter (TSP, PM_{10} and $PM_{2.5}$), hydrogen sulphide, total reduced sulphur and sulphur dioxide.

On Monday, March 14, 2005 at approximately 9:45am, a release occurred from a ruptured storage vessel at the Shell Chemicals Scotford site, northeast of Edmonton. The release consisted of a mixture of styrene and ethylbenzene, which escaped from a storage tank and resulted in a vapour release that moved offsite[3]. Alberta Environment's mobile lab was deployed to the Scotford site and arrived shortly after 12:00pm; monitoring began at 12:25pm. The MAML was not designed or equipped for emergency response monitoring, however, it can be used in a limited capacity to provide such support during upset conditions.

Alberta Environment enhanced the MAML's suite of analyzers prior to arriving at the Scotford site with the addition of a MIRAN SapphIRe Portable Ambient Air Analyzer; the unit was on loan to Alberta Environment to evaluate its performance. The SapphIRe unit uses spectroscopic technology, a technique that is based on the interaction of energy with a sample of air to perform analysis[2]. Infrared spectophotometry involves the absorption of infrared light which occurs at a specific wavelength for individual compounds. By selecting different wavelengths, it is possible to monitor for specific volatile organic compounds (VOCs). The SapphIRe unit is not considered a continuous analyzer and it is primarily used to measure concentration 'snap shots' for specific compounds[4].

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Alberta Environment has not yet validated the infrared technology of the SapphIRe unit. The unit's vendor has data that verifies its accuracy however, Alberta Environment has not completed the rigorous testing required to qualify this instrument as a compliance air monitoring tool. Alberta Environment does not have any immediate plans to permanently install such an instrument on the MAML or to make one available for other air quality monitoring projects.

All of the monitoring locations were offsite and generally downwind from the Scotford Complex. Monitoring sites were selected based on wind direction, plume movement and road accessibility. 1-hour Alberta Ambient Air Quality Objectives (AAAQOs) do not apply to several of the monitoring datasets because the mobile lab was not stationary long enough for comparison to applicable Objectives.

Alberta Environment collected 411 minutes of air quality data with the MAML's standard suite of analyzers and 180 minutes on the SapphIRe unit. This report presents hydrocarbon (total hydrocarbons, reactive hydrocarbons, methane and polycyclic aromatic hydrocarbons), and VOC (styrene and ethylbenzene) monitoring results.

ISBN: 0-7785-4047-2 (Printed)
ISBN: 0-7785-4232-7 (On-line)
Pub No. T/811
May 17, 2005

Findings

(1) In typical pro-active surveys, the MAML is stationary for a period of time long enough to compare measured concentrations to 1-hour Alberta Ambient Air Quality Objectives (AAAQOs). During this emergency response event, the lab was generally mobile around the perimeter of the Shell Scotford Complex and nearby communities. Concentrations of selected air pollutants measured during the March 14, 2005 Shell Chemicals release (the Upset) can be found in Table 1. The concentrations presented in Table 1 are overall summary statistics for the whole dataset. In non-emergency response reports, the 'median' column for example, would present the median 1-hour average concentration.

Table 1: Summary of MAML Monitoring results for the Shell Chemicals Upset.

Pollutant	Units	Minimum	Median	Maximum
Hydrocarbons – Methane **(CH_4)**	ppm	2.6	3.0	6.3
Hydrocarbons – Reactive Hydrocarbons **(RHC)**	ppm	bd	bd	6.7
Hydrocarbons – Total Hydrocarbons **(THC)**	ppm	2.7	3.1	10.4
Hydrocarbons – Polycyclic Aromatic Hydrocarbons **(PAH)**	ng/m^3	bd	bd	55
Individual Volatile Organic Compound – Styrene **(C_8H_{10})**	ppm	bd	bd	2.5
Individual Volatile Organic Compound – Ethylbenzene **($C_6H_5CH=CH_2$)**	ppm	bd	5.6	7.9

ppm – parts per million ng/m^3 – nanograms per cubic meter of air bd – below detection limit

(2) The highest hydrocarbon concentrations were measured on perimeter roadways surrounding the Scotford complex and near the main plant gate. Elevated hydrocarbon concentrations at these locations may be attributed to the vapour release from the Upset. The highest methane, total hydrocarbon and reactive hydrocarbon concentrations were measured at the Scotford Complex main gate. The highest methane concentration of 6.3 ppm was measured at 15:27. The highest total hydrocarbon and reactive hydrocarbon concentrations measured were 10.4 ppm and 6.7 ppm respectively; both of these concentrations were measured at 13:53.

The highest polycyclic aromatic hydrocarbon (PAH) concentration of 55 ng/m^3 was measured at 12:39 while initially tracking the plume on Highway 15. Elevated PAH concentrations at this time and location are likely highway vehicle exhaust emissions.

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The highest polycyclic aromatic hydrocarbon (PAH) concentration of 55 ng/m^3 was measured at 12:39 while initially tracking the plume on Highway 15. Elevated PAH concentrations at this time and location are likely highway vehicle exhaust emissions.

(3) The SapphIRe unit was used to intermittently measure styrene and ethylbenzene concentrations at selected monitoring locations. The lower detection limits (the lowest concentration that the SapphIRe unit can detect) for styrene and ethylbenzene are 0.6 ppm and 1.2 ppm respectively.

(a) The SapphIRe unit has an accuracy of ±15%, as determined by the manufacturer. Although the unit was still being evaluated by monitoring staff, Alberta Environment was fortunate to have the SapphIRe unit available to monitor for potentially high concentrations of selected compounds during the Upset. It should be noted that the SapphIRe unit was not challenged with appropriate verification gases prior to, or after use during the Upset. Therefore, styrene and ethylbenzene results should not be considered absolute but rather indicative of whether ambient concentrations were above what may be considered background levels.

(b) The highest styrene concentration of 2.5 ppm was measured at 14:55 on Range Road 214 approximately 440 meters south of the Scotford Complex main gate. At this location, from 14:49 to 15:13 (25 minutes), Alberta Environment consistently measured concentrations above 1.8 ppm.

(c) The highest ethylbenzene concentration of 7.9 ppm was measured at 14:41 on Range Road 214 approximately 440 meters south of the Scotford Complex main gate. At this location, from 14:27 to 14:47 (18 minutes), Alberta Environment consistently measured concentrations above 7.6 ppm.

The Mobile Air Monitoring Laboratory (MAML)

The MAML is a 27-foot (8.2 meters) vehicle that has been specially designed and equipped to measure air quality. It houses a variety of instruments that continuously sample the air at specified time or distance intervals. The MAML is equipped with:

- a dual computer system custom-programmed to accept and record the measurement of air samples from each analyser,
- a GPS (Global Positioning System) that identifies the MAML's location as it moves around Alberta,
- an exhaust purifying system that minimizes emissions from the vehicle
- two on-board generators that are also equipped with exhaust scrubbers

The pollutants that the MAML are capable of monitoring are listed in Table 3.

Figure 1: **Alberta Environment's Mobile Air Monitoring Laboratory**

Table 2 **Pollutants that the MAML is capable of monitoring (including minimum detection limits and operating ranges).**

Pollutant	Operating Range	
	Lower Detection Limit*	Upper Detection Limit**
Ammonia **(NH_3)**	0.001 ppm	5 ppm
Carbon Monoxide **(CO)**	0.1 ppm	50 ppm
Hydrocarbons – Methane **(CH_4)**	0.1 ppm	10 ppm
Hydrocarbons – Reactive Hydrocarbons **(RHC)**	0.1 ppm	20 ppm
Hydrocarbons – Total Hydrocarbons **(THC)**	0.1 ppm	20 ppm
Hydrocarbons – Polycyclic Aromatic Hydrocarbons **(PAH)**	3 ng/m^3	1000 ng/m^3
Nitrogen dioxide **(NO_2)**	0.001 ppm	1 ppm
Nitric Oxide **(NO)**	0.001 ppm	1 ppm
Oxides of nitrogen **(NO_x)**	0.001 ppm	1 ppm
Ozone **(O_3)**	0.001 ppm	0.5 ppm
Particulates – Total Suspended Particulates **(TSP)**	1 $\mu g/m^3$	1.0 g/m^3
Particulates – Particulate Matter <10μm **(PM_{10})**	1 $\mu g/m^3$	1.0 g/m^3
Particulates – Particulate Matter <2.5μm **($PM_{2.5}$)**	1 $\mu g/m^3$	1.0 g/m^3
Sulphur Compounds - Hydrogen Sulphide **(H_2S)**	0.001 ppm	1 ppm
Sulphur Compounds - Total Reduced Sulphur **(TRS)**	0.001 ppm	1 ppm
Sulphur Dioxide **(SO_2)**	0.001 ppm	1 ppm
*Individual Volatile Organic Compound*** – Styrene **(C_8H_{10})**	0.6 ppm	200 ppm
*Individual Volatile Organic Compound*** – Ethylbenzene **($C_6H_5CH=CH_2$)**	1.2 ppm	200 ppm

ppm - parts per million

ng/m^3 = nanograms per cubic metre

$\mu g/m^3$ = micrograms per cubic metre

g/m^3 = grams per cubic metre

* The ***lower detection limit*** indicates the *minimum* amount of pollutant and the lower limit of meteorological data can be measured by the instrument.

** The ***upper detection limit*** indicates the *maximum* amount of pollutant the instrument can detect and the upper limit for meteorological data measured. This limit is set to provide the optimum precision over that range. The upper limit can be raised, however, precision at the lower levels (where most levels are monitored) is then compromised.

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Nitric Oxide **(NO)**	0.001 ppm	1 ppm
Oxides of nitrogen **(NO_x)**	0.001 ppm	1 ppm
Ozone **(O_3)**	0.001 ppm	0.5 ppm
Particulates – Total Suspended Particulates **(TSP)**	1 $\mu g/m^3$	1.0 g/m^3
Particulates – Particulate Matter <10µm **(PM_{10})**	1 $\mu g/m^3$	1.0 g/m^3
Particulates – Particulate Matter <2.5µm **($PM_{2.5}$)**	1 $\mu g/m^3$	1.0 g/m^3
Sulphur Compounds - Hydrogen Sulphide **(H_2S)**	0.001 ppm	1 ppm
Sulphur Compounds - Total Reduced Sulphur **(TRS)**	0.001 ppm	1 ppm
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Monitoring Method and Locations

Alberta Environment used the MAML to monitor pollutant concentrations around the Scotford Complex. The monitoring sites were selected based on wind direction (See Figure 4), plume movement and road accessibility. MAML monitoring locations are presented in Figure 2, described in Table 3, and depicted in Figure 3.

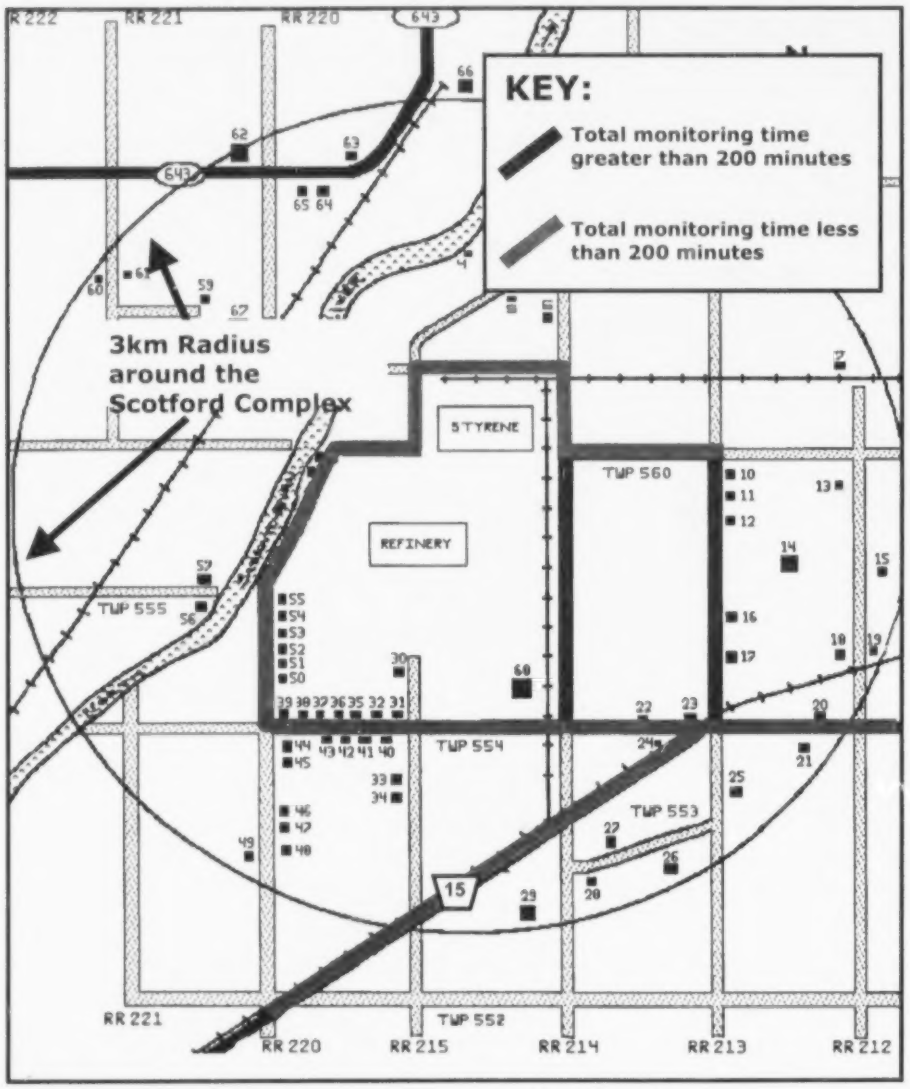

Figure 2: **Locations and routes monitored by the MAML.**

Adapted from: Scotford Styrene Approval No. 002-9767

Table 3: Locations monitored by the MAML on March 14, 2005.

Dataset Name	Monitoring Location or Route Description	Time	Duration
SHELL1	Mobile on Highway 15 between Range Roads 211 and 214	12:28 – 13:22 (mobile)	55 minutes
SHELL2	Shell Chemicals Main Gate	13:27 – 14:07 (stationary)	60 minutes
	80 meters south of Shell Chemicals Main Gate	14:08 – 14:26 (stationary)	
SHELL3	40 meters south of Shell Chemicals Main Gate	14:27 – 15:21 (stationary)	60 minutes
	Shell Chemicals Main Gate	15:23 – 15:26 (stationary)	
SHELL4	Depart main gate, travel east on Township Road 560, then south on Range Road 213	15:27 – 15:44 (mobile)	45 minutes
	Stop at residence 55523 on Range Road 213	15:45 – 16:03 (stationary)	
	Stop at residence 55447 on Range Road 213	16:07 – 16:08 (stationary)	
	Travel south on Range Road 213 to Highway 15	16:09 – 16:11 (mobile)	
SHELL5	East on Highway 15	16:12 (mobile)	21 minutes
	Stop at Tempo Gas Station on Highway 15	16:13 – 16:29 (stationary)	
	Depart Tempo Gas Station and travel west on Highway 15 then north on Range Road 213	16:30 – 16:32 (mobile)	
SHELL6	Travel West on Township Road 554	16:34 (mobile)	10 minutes
	Stop at residence 21323 on Township Road 554	16:36 – 16:38 (stationary)	
	Depart residence and continue west on Township Road 554 then north on Range Road 214	16:39 – 16:45 (mobile)	
SHELL7	Travel north very slowly on Range Road 214	16:46 – 17:01 (mobile)	16 minutes
SHELL8	Stop 460 meters south of Main Gate on Range Road 214	17:02 – 17:52 (stationary)	53 minutes
	Travel North to Main Gate, then U-turn, travel south on Range Road 214	17:53 – 17:54 (mobile)	
SHELL9	Continue south on Range Road 214	17:56 – 18:03 (mobile)	16 minutes
	Turn onto Township Road 554 and continue west	18:04 – 18:11 (mobile)	
SHELL10	Stop 400 meters west of Range Road 214 on Township Road 554	18:11 – 18:37 (stationary)	75 minutes
	Travel west on Township Road 554 then north on Range Road 220 to complete circle around Styrene plant	18:38 – 19:17 (mobile)	
	South on Range Road 214 past Main Gate. End Monitoring.	19:18 – 19:24 (mobile)	

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	Shell Chemicals Main Gate	15:23 – 15:26 (stationary)	
SHELL4	Depart main gate, travel east on Township Road 560, then south on Range Road 213	15:27 – 15:44 (mobile)	45 minutes
	Stop at residence 55523 on Range Road 213	15:45 – 16:03 (stationary)	
	Stop at residence 55447 on Range Road 213	16:07 – 16:08 (stationary)	
	Travel south on Range Road 213 to Highway 15	16:09 – 16:11 (mobile)	
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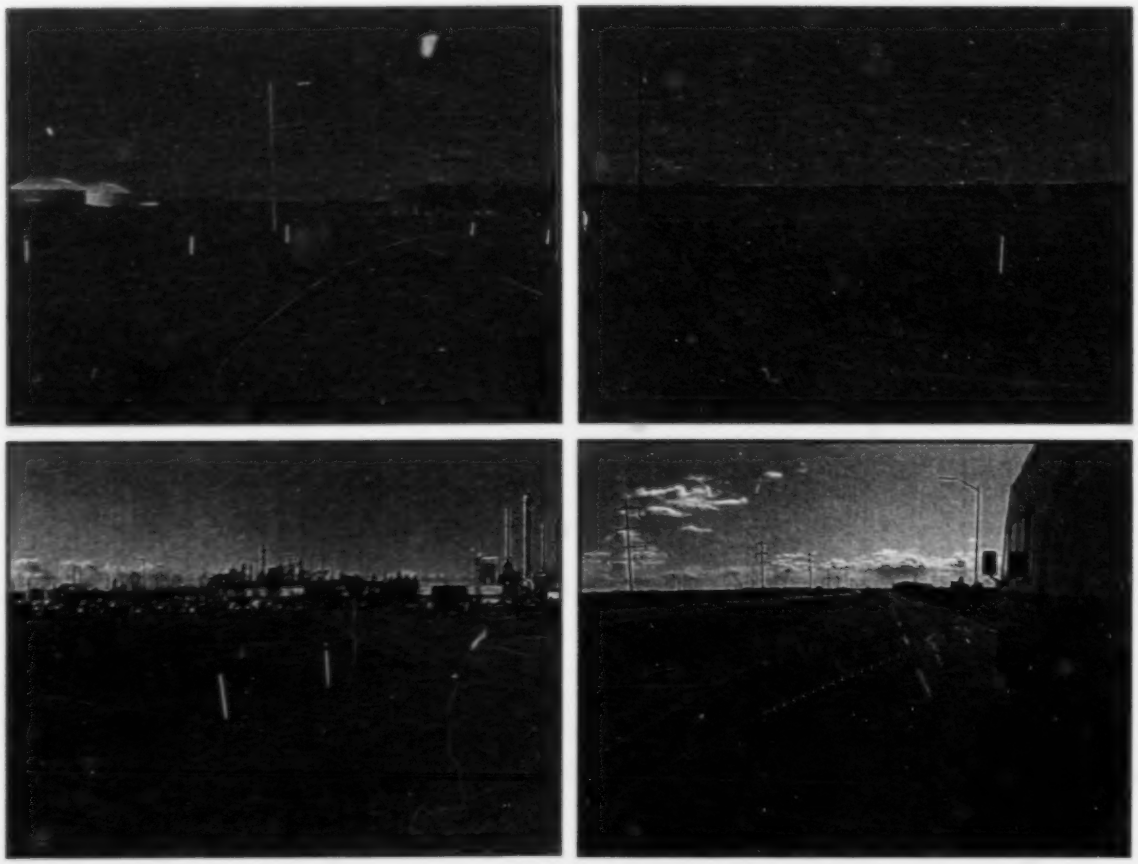

Figure 3: **Clockwise from upper left: north, east, south and west views of the monitoring location near the Scotford Complex Main Gate on Range Road 214 (March 14, 2005 at 14:47).**

Wind direction during the Upset was predominantly from the northwest and north northwest; most monitoring was conducted southeast of the Scotford Complex on Range Roads 213 and 214. Wind direction and wind speed were measured only while the MAML was stationary.

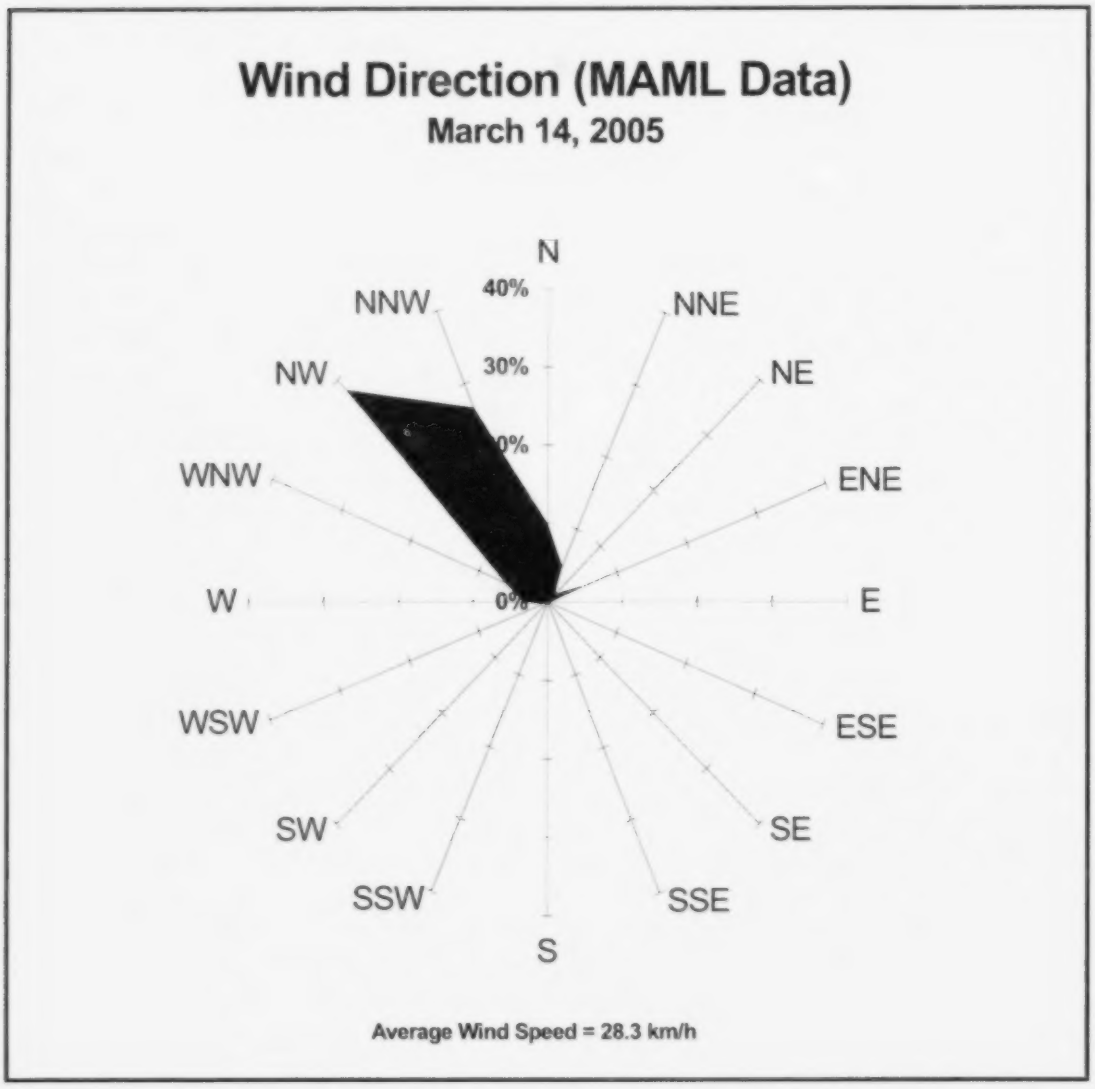

Figure 4: **Wind rose plot for all wind direction data collected by the MAML on March 14, 2005.**

Results

The maximum concentration is the highest concentration measured for the given location and monitoring period. The median concentration is a common way of representing the central value for environmental data. Most environmental data usually consist of a distribution that is skewed to the right; that is most data values are low and only a few are high. The arithmetic mean will be biased by the high concentrations and will reveal a value that may not be representative of the central value for the data set. The median is the middlemost value in the data set, dividing the distribution into two equal halves. Therefore, the median is more representative of the central value of a data distribution.

For example, consider a data distribution consisting of five numbers: 1, 2, 2, 3 and 10. The arithmetic mean of these data is 3.6 and the median is 2. In this case, the arithmetic mean is biased high by the extreme value of 10. The median value is actually a true central value of the data distribution.

Many areas in Alberta are pristine and certain pollutants that Alberta Environment monitors for are found in concentrations below the lower detection limit of the instruments onboard the MAML. Consider a dataset that contains 4 concentrations below the detection limit and 1 concentration within the operating range of the MAML instruments; with this data set, it is possible to have an overall median concentration that is 'undetectable' or below the lower detection limit while still having a 'detectable' maximum value.

In the following sections, the monitoring results are presented on column graphs. The following diagram explains how to interpret the results in the following section:

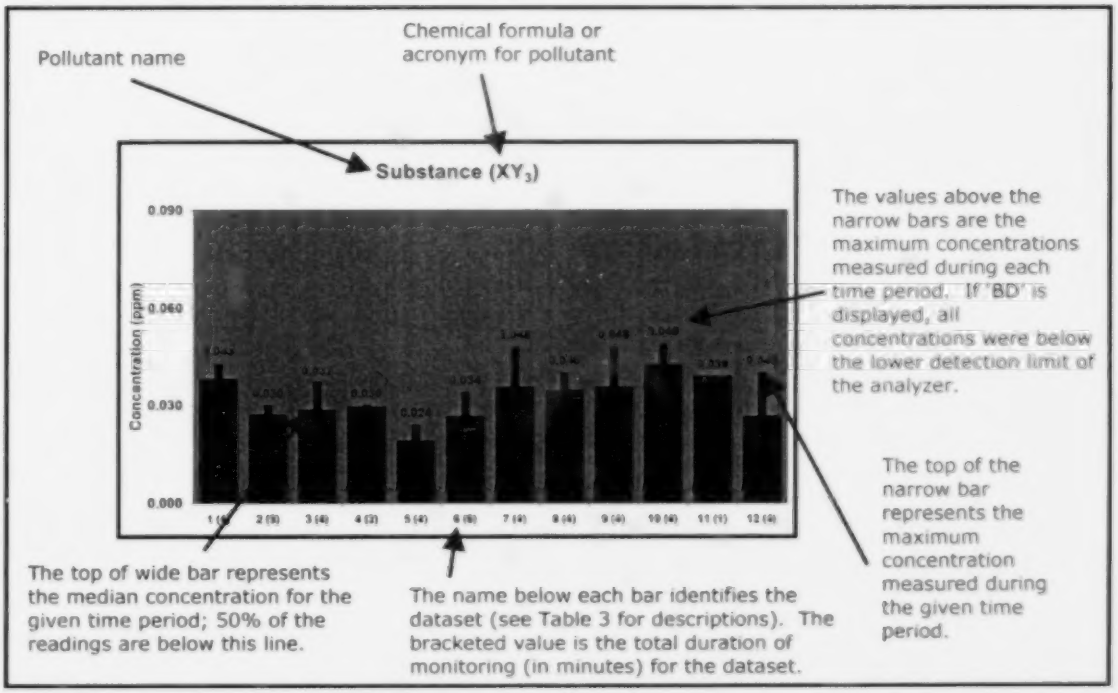
Pollutant name
Chemical formula or acronym for pollutant
Substance (XY_3)
Concentration (ppm)
0.090
0.060
0.030
0.000
The values above the narrow bars are the maximum concentrations measured during each time period. If 'BD' is displayed, all concentrations were below the lower detection limit of the analyzer.
The top of the narrow bar represents the maximum concentration measured during the given time period.
The top of wide bar represents the median concentration for the given time period; 50% of the readings are below this line.
The name below each bar identifies the dataset (see Table 3 for descriptions). The bracketed value is the total duration of monitoring (in minutes) for the dataset.

Figure 5: Graph interpretation key.

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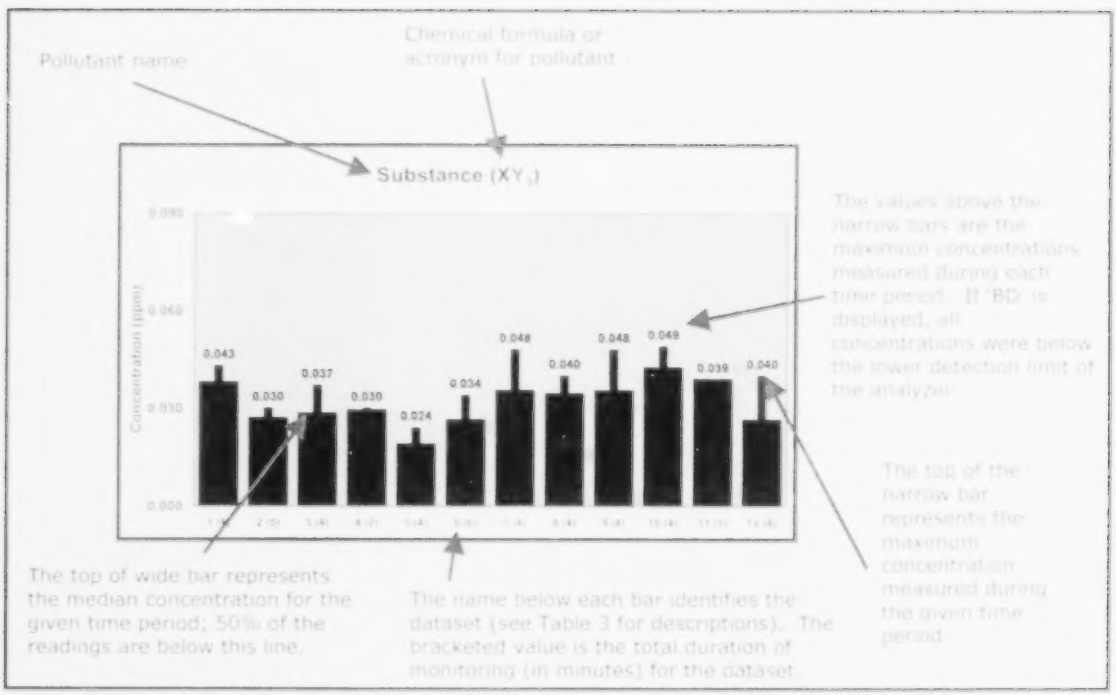
Pollutant name
Chemical formula or acronym for pollutant
Substance (XY_3)
Concentration (ppm)
0.060
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0.000
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0.030
0.037
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Hydrocarbons (CH_4, RHC, THC, PAHs)

The term "total hydrocarbons" (THC) refers to a broad family of chemicals that contain carbon and hydrogen atoms. Methane (CH_4) is the most common natural hydrocarbon in the earth's atmosphere. Reactive hydrocarbons (RHC) are important because they can contribute to summertime smog or be toxic at high concentrations. Some sources of hydrocarbons include vegetation, vehicle emissions, oil and gas processing, chemical processing, dry cleaning, fireplaces, natural gas combustion, aircraft traffic and evaporation of solvents.

Polycyclic aromatic hydrocarbons (PAHs) are a class of chemicals that are usually contained in soot and smoke. There are more than 100 different PAHs with varying levels of toxicity. They are formed during the incomplete combustion of gasoline, diesel, oil, coal, wood, garbage or other organic substances. Tobacco smoke and charbroiled meats are common sources of PAHs. Other outdoor PAH sources include vehicle emissions, wood smoke from fireplaces, smoke from forest fires and industrial facilities. PAHs occur in the atmosphere in the vapour phase or attached to dust particles.

The highest concentrations of hydrocarbons were measured on perimeter roadways surrounding the Scotford complex and near the main plant gate. Elevated hydrocarbon concentrations at these locations may be attributed to the vapour release from the Upset.

On the following graphs, the columns for the SHELL2, SHELL3, SHELL4 and SHELL8 datasets have been highlighted in blue because all reactive hydrocarbon concentrations for these groups are notably higher than background concentrations. It is at these locations that the SapphIRe unit was operational and therefore, intermittent styrene and ethylbenzene concentrations were determined. Results of the SapphIRe hydrocarbon analysis are discussed in later sections of this report.

The instrument that analyzes methane was impacted by the particularly elevated reactive hydrocarbon concentrations; methane concentrations for the SHELL2, SHELL3, SHELL4 and SHELL8 datasets are 'artificially high'. The hydrocarbon analyzer measures methane by scrubbing out other hydrocarbons and allowing methane to "pass through" for analysis. The scrubbing system is not 100% efficient; this is especially a problem if reactive hydrocarbons concentrations are extremely high. Therefore, during the Upset, elevated methane concentrations may be the result of small amounts of non-methane components passing through the scrubber system and subsequently being measured as methane.

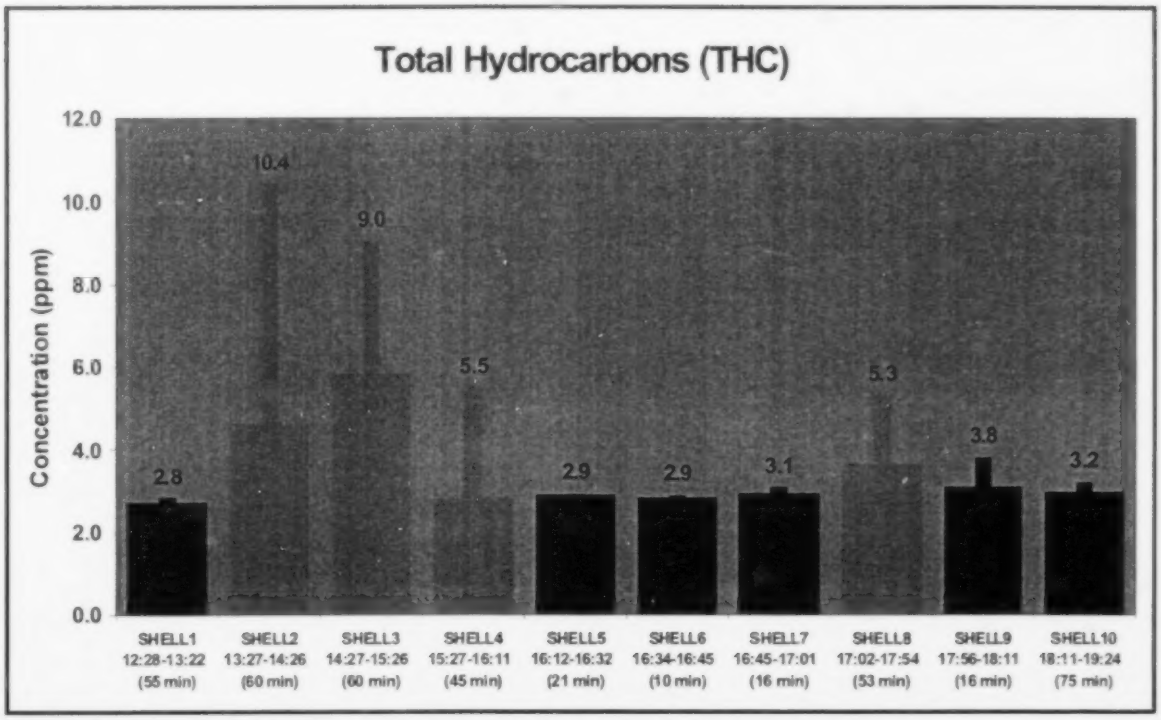


Figure 6: **Median and maximum concentrations for total hydrocarbons.**

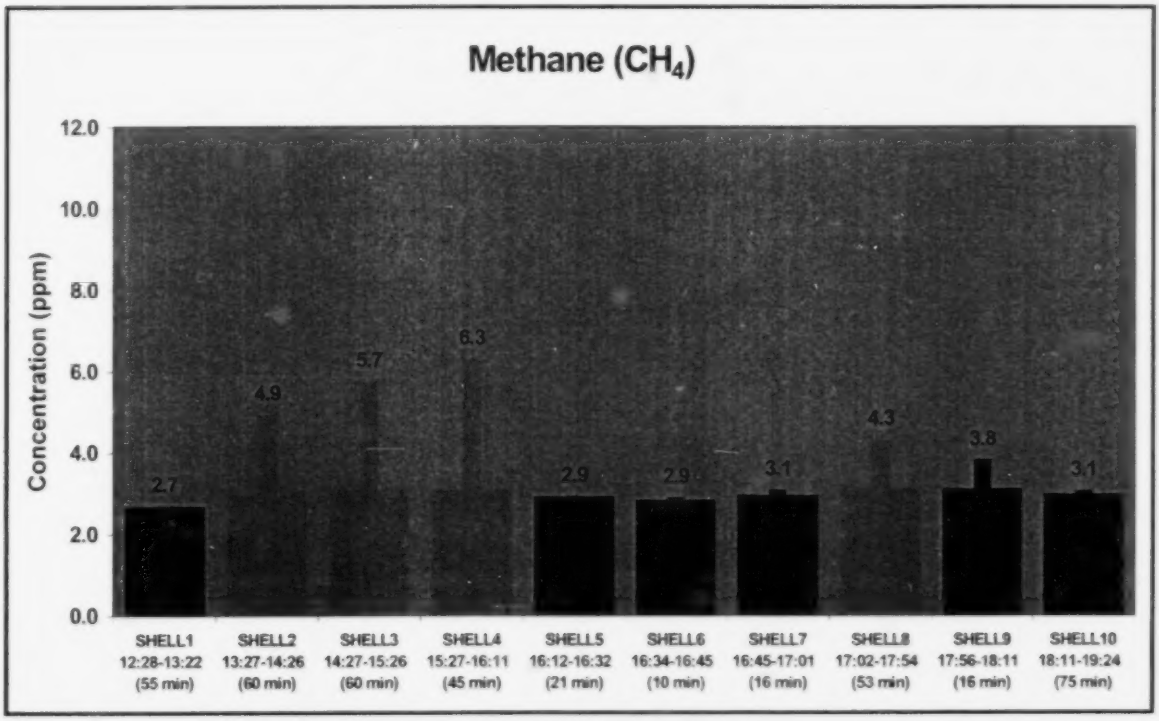


Figure 7: **Median and maximum concentrations for methane.**

Hydrocarbons (CH_4, RHC, THC, PAHs)

The term "total hydrocarbons" (THC) refers to a broad family of chemicals that contain carbon and hydrogen atoms. Methane (CH_4) is the most common natural hydrocarbon in the earth's atmosphere. Reactive hydrocarbons (RHC) are important because they can contribute to summertime smog or be toxic at high concentrations. Some sources of hydrocarbons include vegetation, vehicle emissions, oil and gas processing, chemical processing, dry cleaning, fireplaces, natural gas combustion, aircraft traffic and evaporation of solvents.

Polycyclic aromatic hydrocarbons (PAHs) are a class of chemicals that are usually contained in soot and smoke. There are more than 100 different PAHs with varying levels of toxicity. They are formed during the incomplete combustion of gasoline, diesel, oil, coal, wood, garbage or other organic substances. Tobacco smoke and charbroiled meats are common sources of PAHs. Other outdoor PAH sources include vehicle emissions, wood smoke from fireplaces, smoke from forest fires and industrial facilities. PAHs occur in the atmosphere in the vapour phase or attached to dust particles.

The highest concentrations of hydrocarbons were measured on perimeter roadways surrounding the Scotford complex and near the main plant gate. Elevated hydrocarbon concentrations at these locations may be attributed to the vapour release from the Upset.

On the following graphs, the columns for the SHELL2, SHELL3, SHELL4 and SHELL8 datasets have been highlighted in blue because all reactive hydrocarbon concentrations for these groups are notably higher than background concentrations. It is at these locations that the SapphIRe unit was operational and therefore, intermittent styrene and ethylbenzene concentrations were determined. Results of the SapphIRe hydrocarbon analysis are discussed in later sections of this report.

The instrument that analyzes methane was impacted by the particularly elevated reactive hydrocarbon concentrations; methane concentrations for the SHELL2, SHELL3, SHELL4 and SHELL8 datasets are 'artificially high'. The hydrocarbon analyzer measures methane by scrubbing out other hydrocarbons and allowing methane to "pass through" for analysis. The scrubbing system is not 100% efficient; this is especially a problem if reactive hydrocarbons concentrations are extremely high. Therefore, during the Upset, elevated methane concentrations may be the result of small amounts of non-methane components passing through the scrubber system and subsequently being measured as methane.

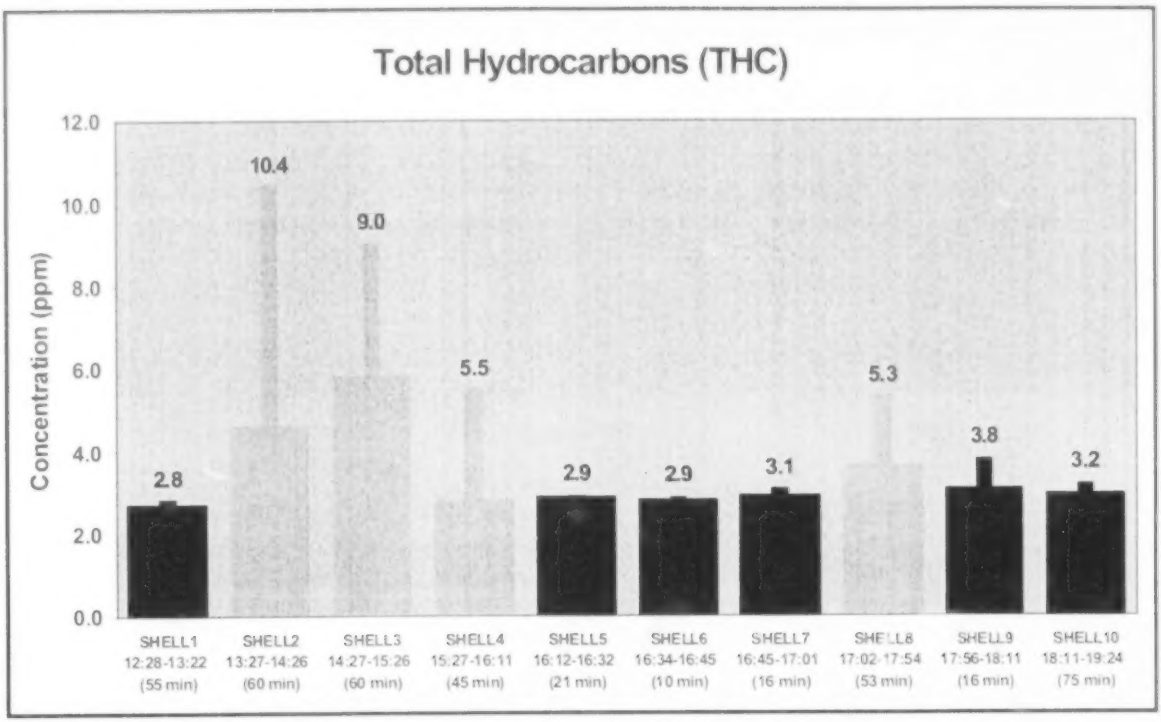


Figure 6: Median and maximum concentrations for total hydrocarbons.

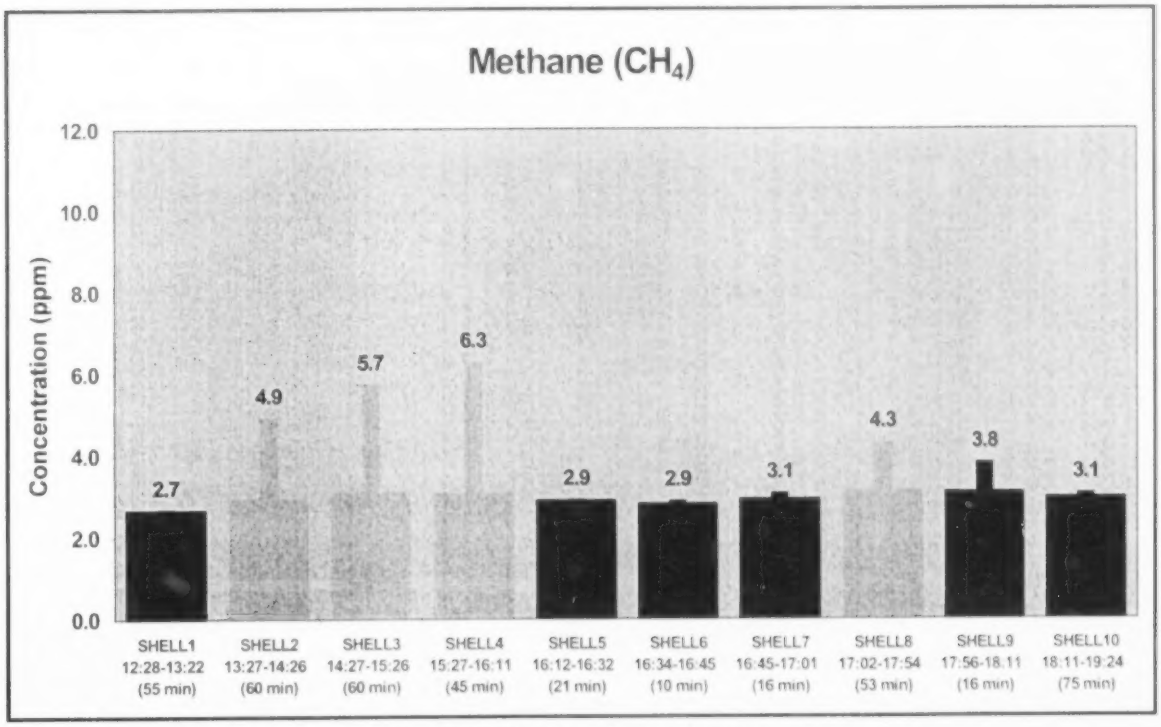


Figure 7: Median and maximum concentrations for methane.

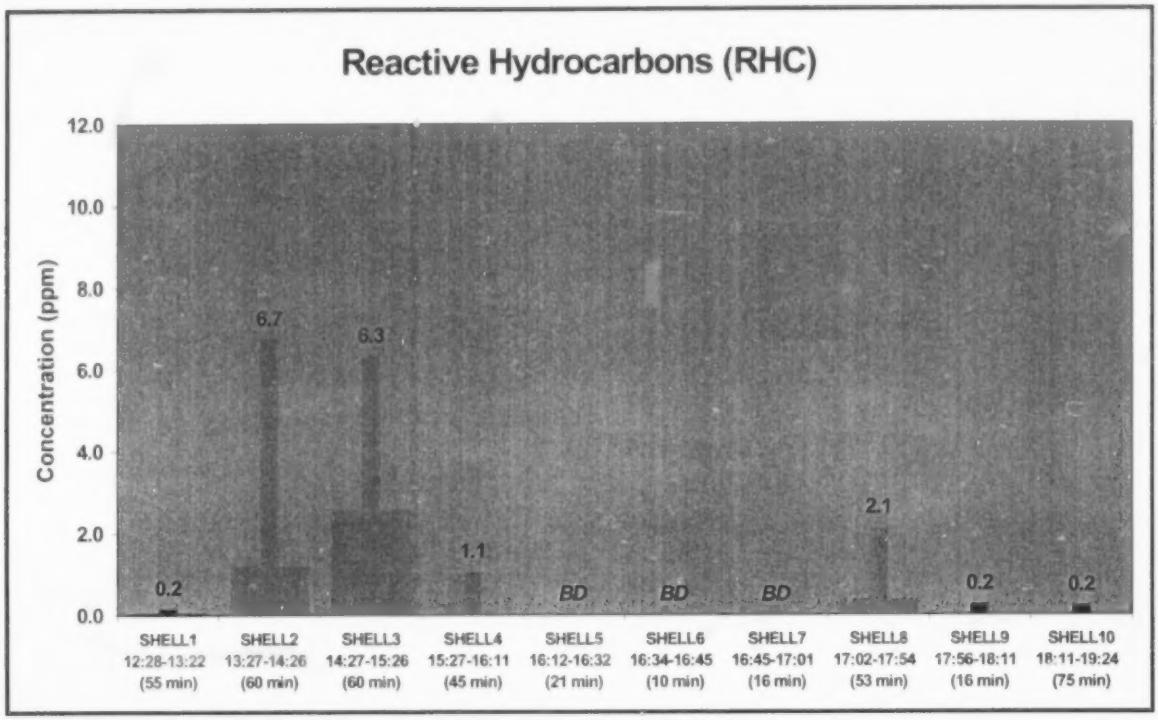


Figure 8: **Median and maximum concentrations for reactive hydrocarbons.**

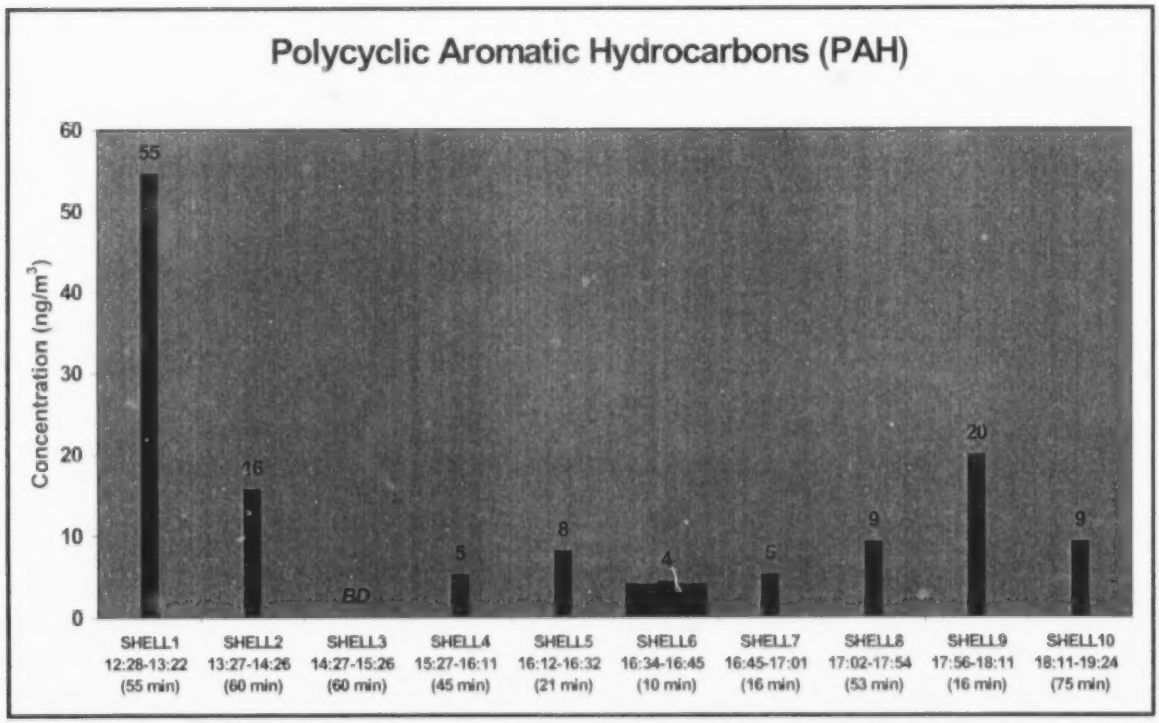


Figure 9: **Median and maximum concentrations for polycyclic aromatic hydrocarbons.**

Volatile Organic Compounds (VOC)

Volatile organic compounds (VOCs) include a large group of chemicals containing carbon and hydrogen atoms that can react quickly to form other chemicals in atmosphere. VOCs are important because they can: (1) react with oxides of nitrogen in the presence of sunlight to form ozone and photochemical smog; and (2) be toxic to humans, animals or vegetation.

The major sources of VOCs are vegetation, automobile emissions, gasoline marketing and storage tanks, petroleum and chemical industries, dry cleaning, fireplaces, natural gas combustion and aircraft. VOC emissions from natural sources, such as forests, grasslands and swamps, are estimated to be almost six times greater than human sources. Individual VOCs are also produced from the evaporation of solvents and organic chemicals as well as from leaking valves, flanges, pumps and compressors at industrial facilities. The major source of VOCs in most urban areas is vehicle exhaust emissions[1].

Alberta Environment enhanced the MAML's suite of analyzers prior to arriving at the Scotford site with the addition of a MIRAN SapphIRe Portable Ambient Air Analyzer. The SapphIRE unit employs spectroscopic technology, a technique that uses the interaction of energy with a sample to perform an analysis. Infrared spectophotometry is based on the absorption of infrared light that occurs at a specific wavelength for individual compounds. By the selection of different wavelengths, it is possible to monitor for a wide range of volatile organic compounds (VOCs). It should be noted that the terms 'reactive hydrocarbons (RHC)' and 'VOCs' are often used interchangeably and both generally refer to the group of substances that form during combustion and evaporation of solvents and fuels. These substances react with oxides of nitrogen in the presence of sunlight to form ozone and photochemical smog.

The SapphIRe unit performs analysis by sending a beam of infrared energy at a selected wavelength through a sample of ambient air; it determines the concentration of selected organic compounds by measuring how much infrared energy passes through the sample. Pollutant concentrations determined by the SapphIRe unit are derived by comparing infrared analysis of the air sample to a library of spectra or 'fingerprints' of different VOCs. Although the SapphIRe unit can measure ambient concentrations of several organic substances, the unit Alberta Environment utilized can only provide data for one substance at a time.

The lower detection limits (the lowest concentration that the SapphIRe unit can detect) for styrene and ethylbenzene are 0.6 ppm and 1.2 ppm respectively.

The highest styrene concentration of 2.5 ppm was measured at 14:55 on Range Road 214 approximately 440 meters south of the Scotford Complex main gate. At this location, from 14:49 to 15:13 (25 minutes), Alberta Environment consistently measured concentrations above 1.8 ppm*.

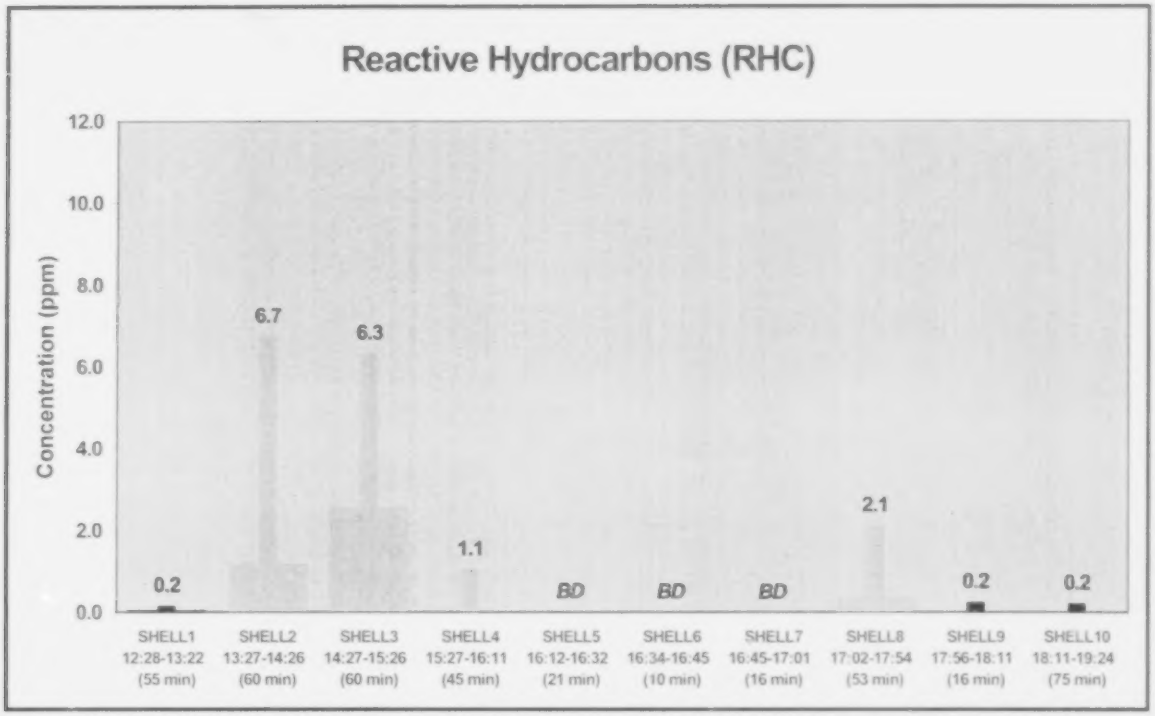


Figure 8: Median and maximum concentrations for reactive hydrocarbons.

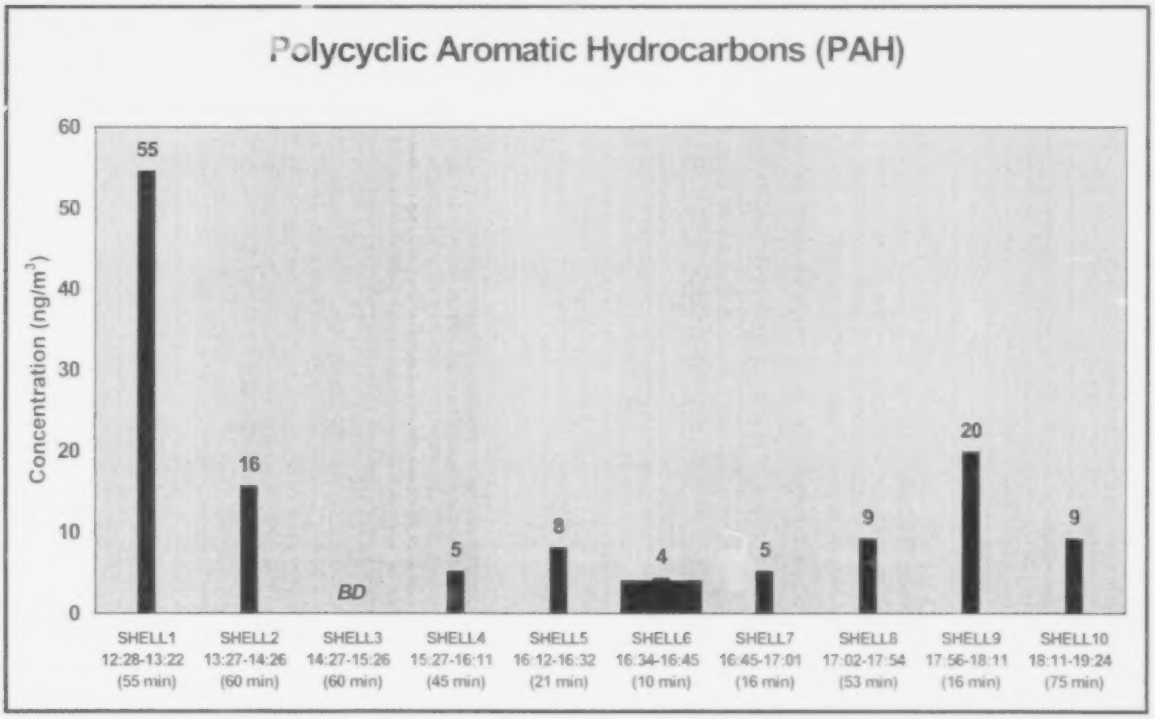


Figure 9: Median and maximum concentrations for polycyclic aromatic hydrocarbons.

Volatile Organic Compounds (VOC)

Volatile organic compounds (VOCs) include a large group of chemicals containing carbon and hydrogen atoms that can react quickly to form other chemicals in atmosphere. VOCs are important because they can: (1) react with oxides of nitrogen in the presence of sunlight to form ozone and photochemical smog; and (2) be toxic to humans, animals or vegetation.

The major sources of VOCs are vegetation, automobile emissions, gasoline marketing and storage tanks, petroleum and chemical industries, dry cleaning, fireplaces, natural gas combustion and aircraft. VOC emissions from natural sources, such as forests, grasslands and swamps, are estimated to be almost six times greater than human sources. Individual VOCs are also produced from the evaporation of solvents and organic chemicals as well as from leaking valves, flanges, pumps and compressors at industrial facilities. The major source of VOCs in most urban areas is vehicle exhaust emissions[1].

Alberta Environment enhanced the MAML's suite of analyzers prior to arriving at the Scotford site with the addition of a MIRAN SapphIRe Portable Ambient Air Analyzer. The SapphIRE unit employs spectroscopic technology, a technique that uses the interaction of energy with a sample to perform an analysis. Infrared spectophotometry is based on the absorption of infrared light that occurs at a specific wavelength for individual compounds. By the selection of different wavelengths, it is possible to monitor for a wide range of volatile organic compounds (VOCs). It should be noted that the terms 'reactive hydrocarbons (RHC)' and 'VOCs' are often used interchangeably and both generally refer to the group of substances that form during combustion and evaporation of solvents and fuels. These substances react with oxides of nitrogen in the presence of sunlight to form ozone and photochemical smog.

The SapphIRe unit performs analysis by sending a beam of infrared energy at a selected wavelength through a sample of ambient air; it determines the concentration of selected organic compounds by measuring how much infrared energy passes through the sample. Pollutant concentrations determined by the SapphIRe unit are derived by comparing infrared analysis of the air sample to a library of spectra or 'fingerprints' of different VOCs. Although the SapphIRe unit can measure ambient concentrations of several organic substances, the unit Alberta Environment utilized can only provide data for one substance at a time.

The lower detection limits (the lowest concentration that the SapphIRe unit can detect) for styrene and ethylbenzene are 0.6 ppm and 1.2 ppm respectively.

The highest styrene concentration of 2.5 ppm was measured at 14:55 on Range Road 214 approximately 440 meters south of the Scotford Complex main gate. At this location, from 14:49 to 15:13 (25 minutes), Alberta Environment consistently measured concentrations above 1.8 ppm*.

The highest ethylbenzene concentration of 7.9 ppm was measured at 14:41 on Range Road 214 approximately 440 meters south of the Scotford Complex main gate. At this location, from 14:27 to 14:47 (18 minutes), Alberta Environment consistently measured concentrations above 7.6 ppm*.

The following maps, wind rose plots and graphs present the styrene and ethylbenzene monitoring results for the SHELL2, SHELL3, SHELL4 and SHELL8 datasets. These datasets were identified in the previous section as having reactive hydrocarbon concentrations significantly above background levels. For each dataset, a map of the monitoring locations, a wind rose plot and a graph showing 1-minute concentrations of selected VOCs are presented.

Presented on the wind rose plots are wind direction data for periods of time that the MAML was stationary; the MAML is not capable of monitoring wind direction or wind speed during mobile monitoring.

** The SapphIRe unit has an accuracy of ±15%, as determined by the manufacturer. The unit was not 'calibrated' or gas challenged prior to, or after use in the Upset; the results may be considered indicative rather than absolute concentrations.*

SHELL2 Dataset

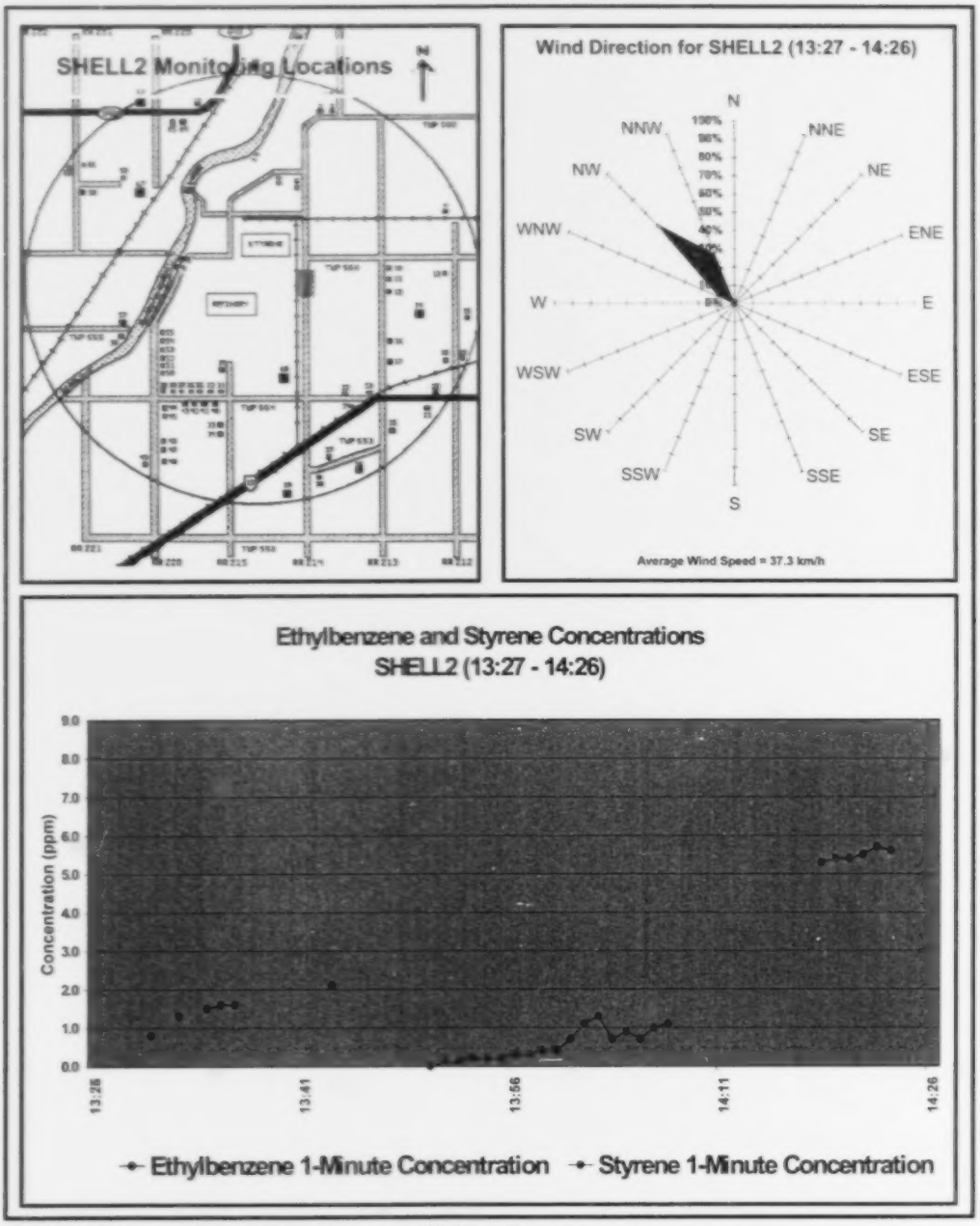
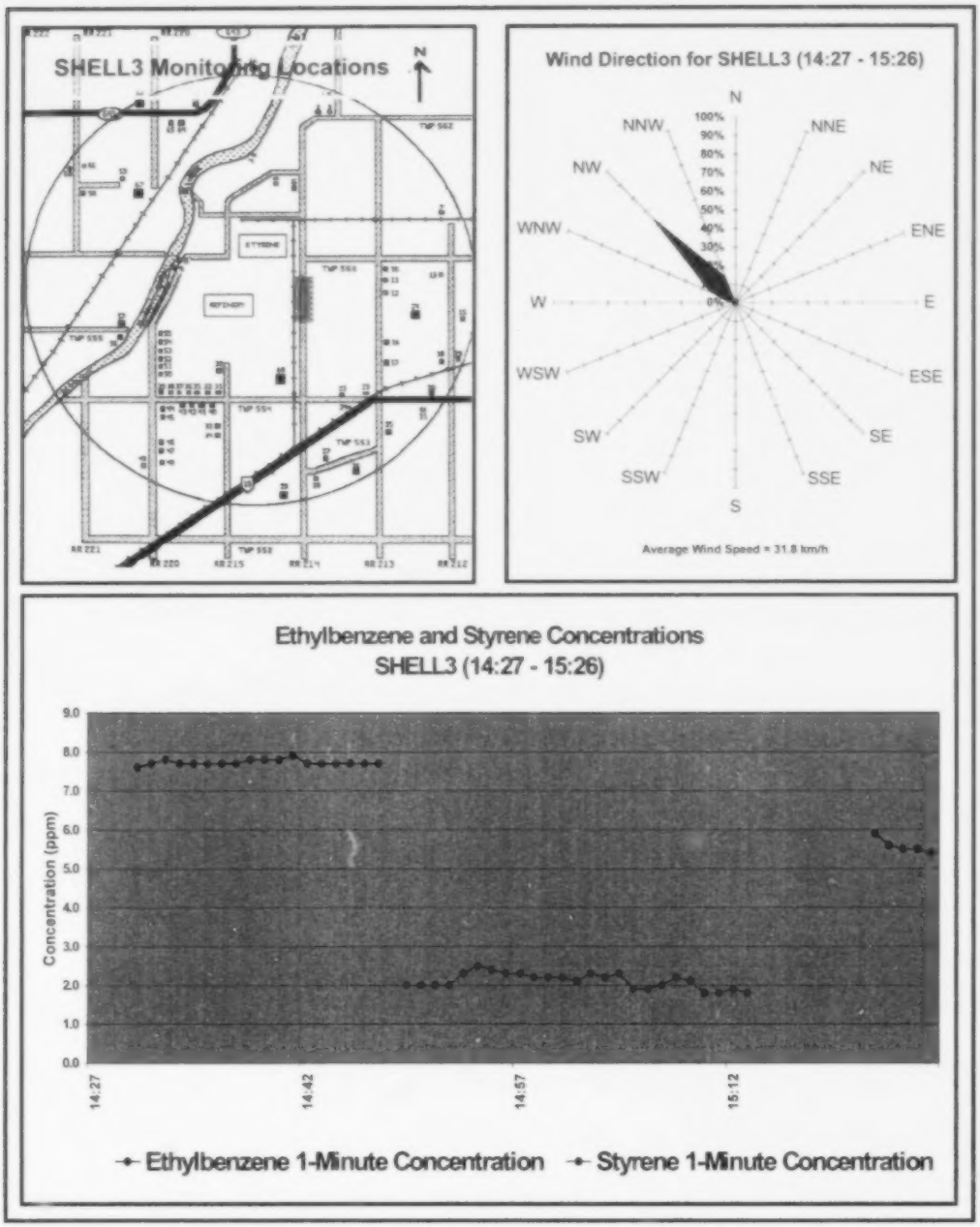


Figure 10: **SHELL2 Dataset reconciliation figures.**

Monitoring Location Notes:

13:27 – 14:07 (stationary)	Shell Chemicals Main Gate
14:08 – 14:26 (stationary)	80 meters south of Shell Chemicals Main Gate

SHELL3 Dataset



Figue 11: **SHELL3 Dataset reconciliation figures.**

Monitoring Location Notes:

14:27 – 15:21 (stationary)	40 meters south of Shell Chemicals Main Gate
14:23 – 15:26 (stationary)	Shell Chemicals Main Gate

SHELL4 Dataset

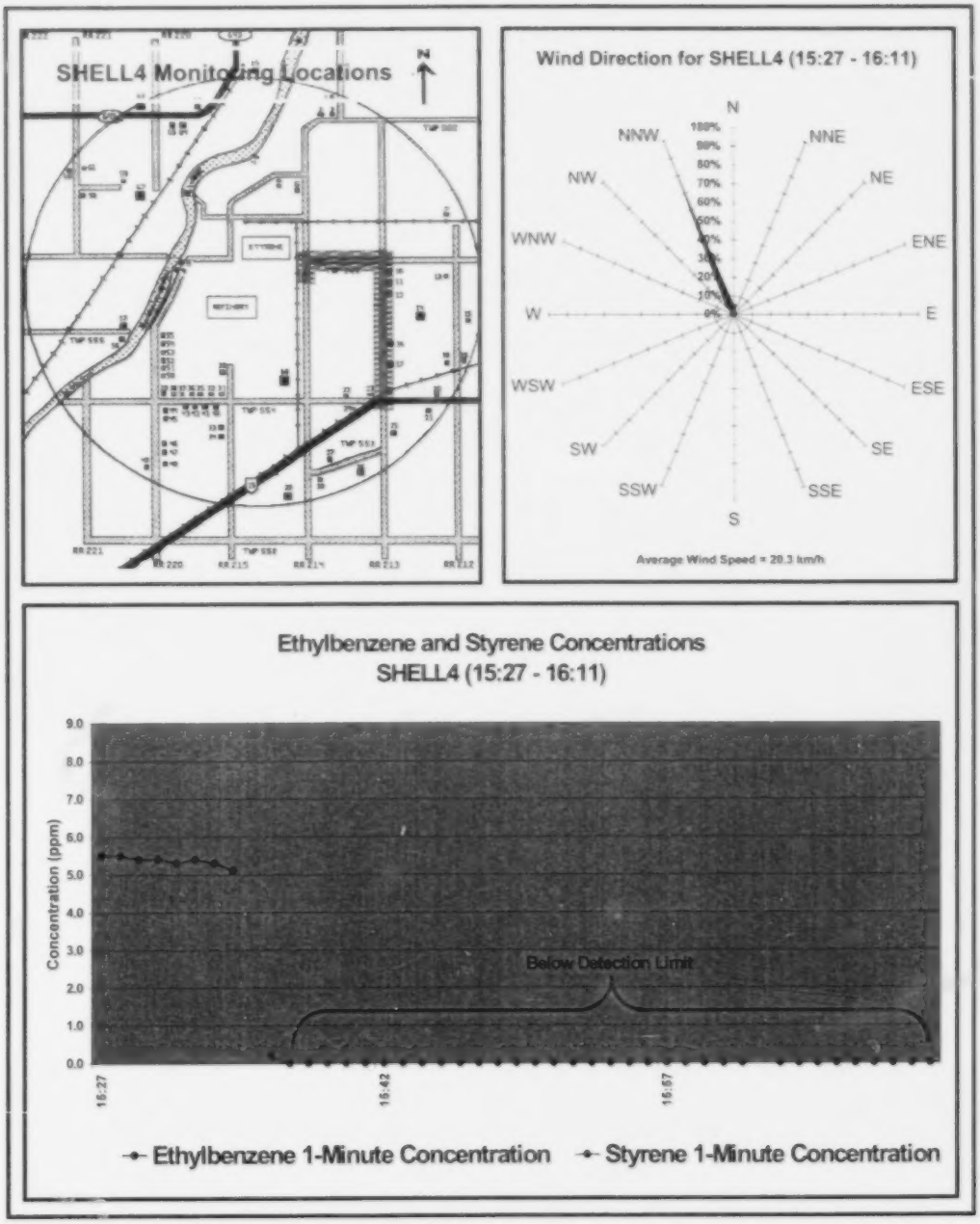


Figure 12: **SHELL4 Dataset reconciliation figures.**

Monitoring Location Notes:

15:27 – 15:44 (mobile)	Depart main gate, travel east on Township Road 560, then south on Range Road 213
15:45 – 16:03 (stationary)	Stop at residence 55523 on Range Road 213
16:07 – 16:08 (stationary)	Stop at residence 55447 on Range Road 213
16:09 – 16:11 (mobile)	Travel south on Range Road 213 to Highway 15

SHELL4 Dataset

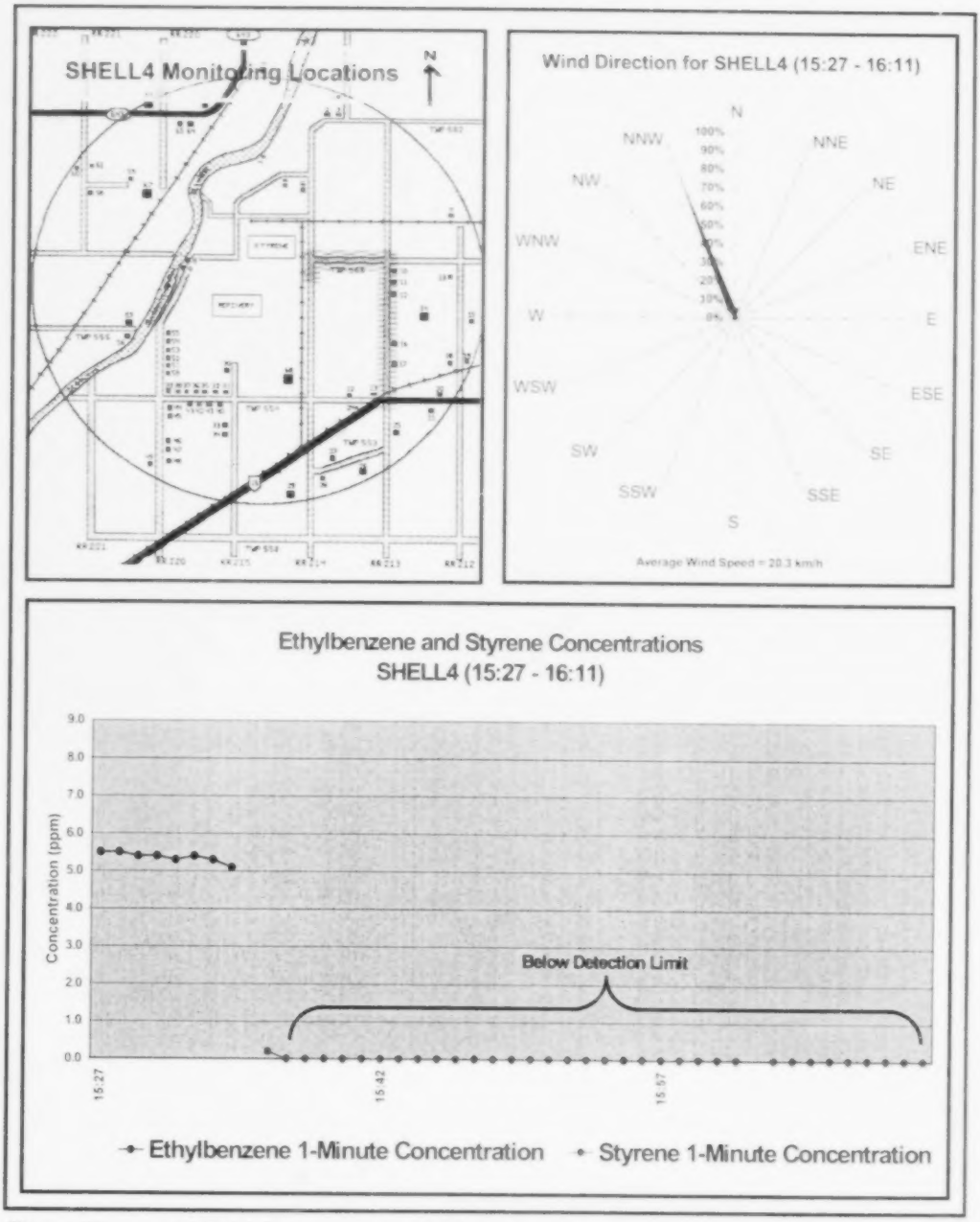


Figure 12: **SHELL4 Dataset reconciliation figures.**

Monitoring Location Notes:

15:27 – 15:44 (mobile)	Depart main gate, travel east on Township Road 560, then south on Range Road 213
15:45 – 16:03 (stationary)	Stop at residence 55523 on Range Road 213
16:07 – 16:08 (stationary)	Stop at residence 55447 on Range Road 213
16:09 – 16:11 (mobile)	Travel south on Range Road 213 to Highway 15

SHELL8 Dataset

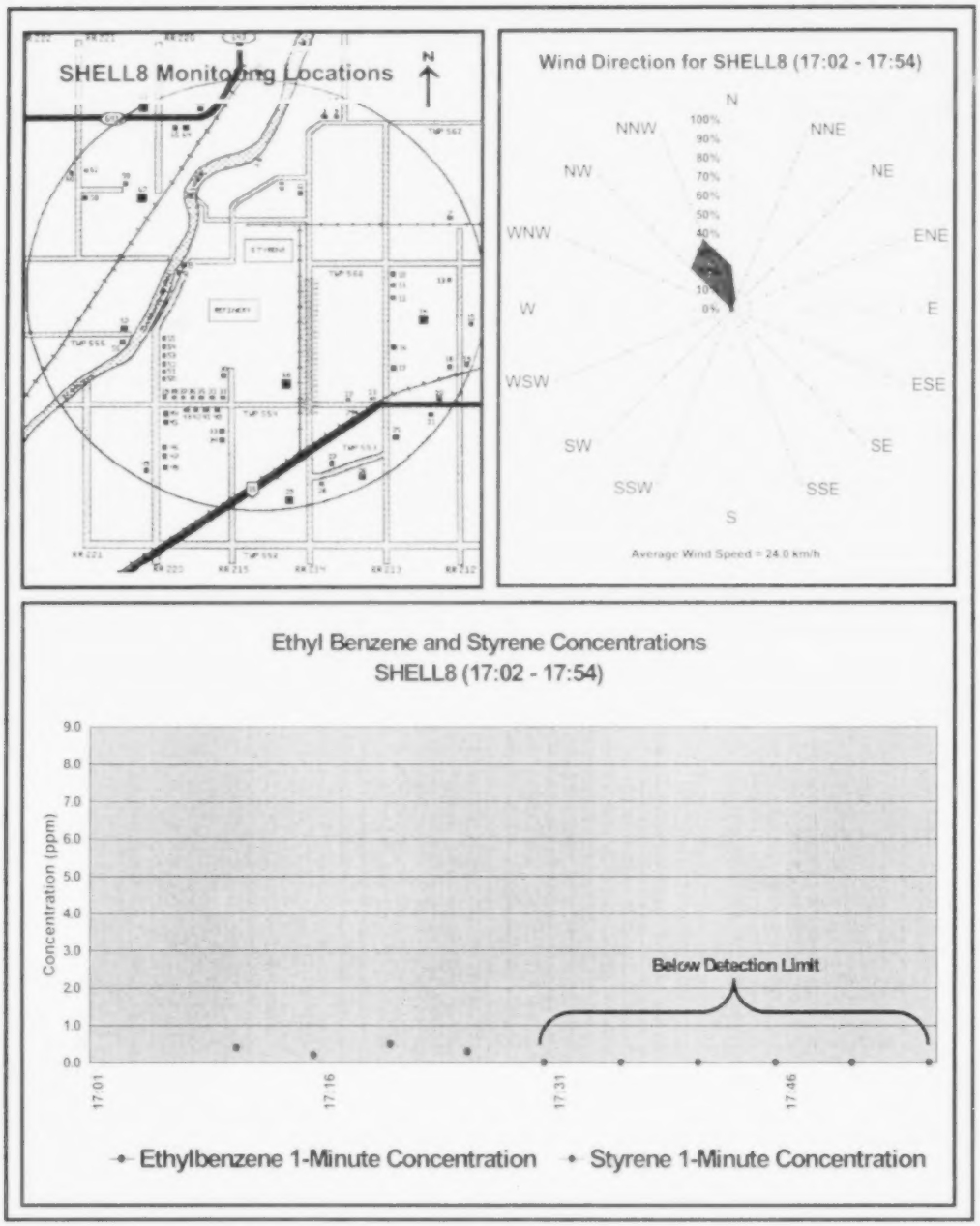


Figure 13: **SHELL8 Dataset reconciliation figures.**

Monitoring Location Notes:

17:02 – 17:52 (stationary)	Stop 460 meters south of Main Gate on Range Road 214
17:53 – 17:54 (mobile)	Travel North to Main Gate, then U-turn, travel south on Range Road 214

SHELL8 Dataset

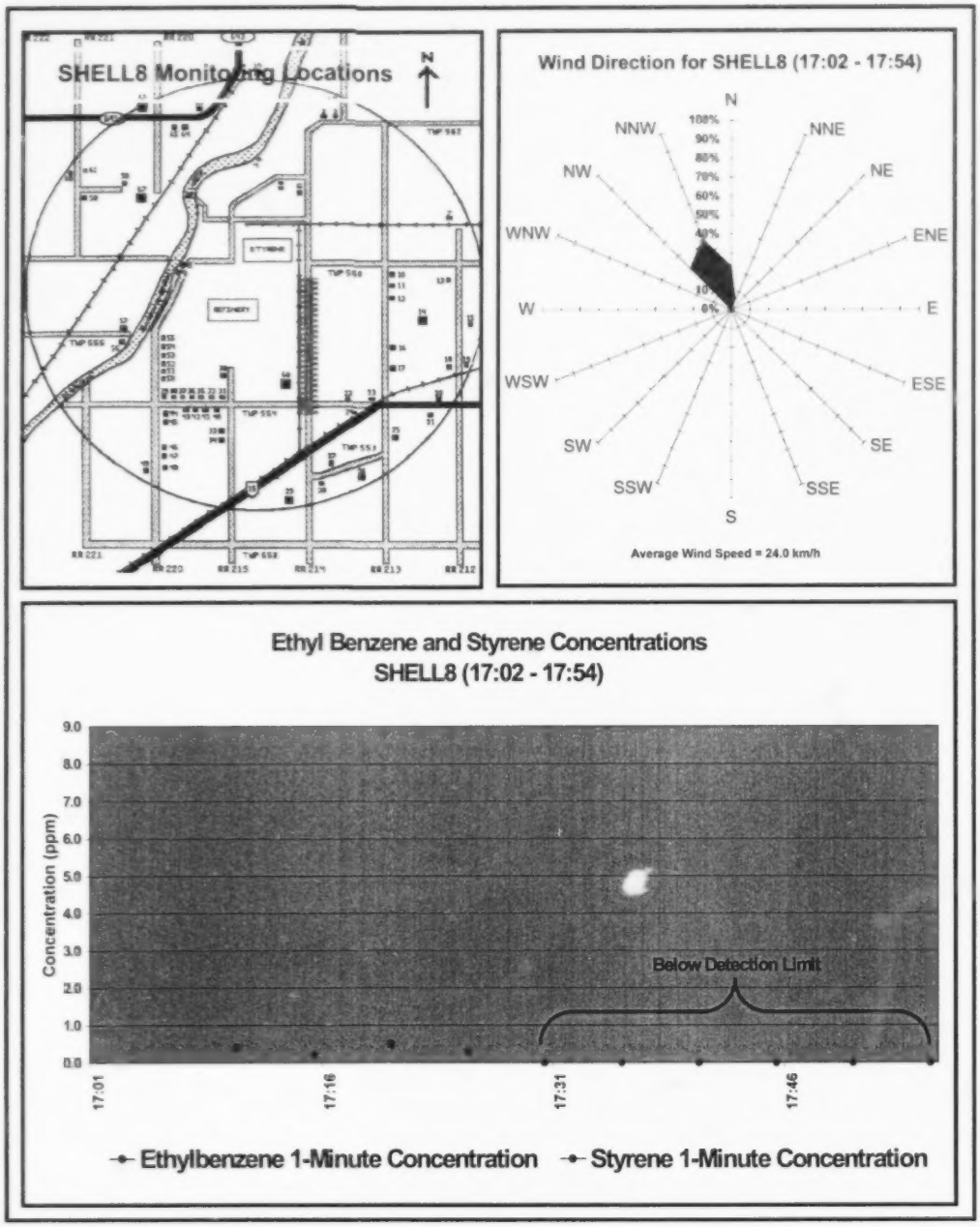


Figure 13: **SHELL8 Dataset reconciliation figures.**

Monitoring Location Notes:

17:02 – 17:52 (stationary)	Stop 460 meters south of Main Gate on Range Road 214
17:53 – 17:54 (mobile)	Travel North to Main Gate, then U-turn, travel south on Range Road 214

Works Cited

1. CASA (Clean Air Strategic Alliance). Substances Monitored, <http://www.casadata.org/pollutants/vol_compounds.asp> January 2005 (Accessed April 1, 2005).

2. Harrop, O.D. 2002, Air Quality Assessment and Management: A Practical Guide, Spon Press, New York.

3. Shell (Shell Chemicals). 2005, Background/Questions and Answers Storage Tank Vapour Release, Shell Chemicals, Fort Saskatchewan.

4. THERMO (THERMO Electron Corporation). 2004, MIRAN 205B Series SapphIRe Portable Ambient Air Analyzers Instruction Manual p/n bk3538, THERMO, Franklin Massachusetts.

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Appendix A

Monitoring Data

Table A1 **Median concentrations measured during the Shell Chemicals Upset.**

				Hydrocarbons				Oxides of Nitrogen				Particulates			Sulphur Compounds		
	Dataset Name	NH_3	CO	CH_4	RHC	THC	PAH	NO_2	NO	NO_X	O_3	TSP	PM_{10}	$PM_{2.5}$	H_2S	TRS	SO_2
		ppm	ppm	ppm	ppm	ppm	ng/m³	ppm	ppm	ppm	ppm	µg/m³	µg/m³	µg/m³	ppm	ppm	ppm
1.	SHELL1	bd	0.035	2.7	bd	2.7	bd	0.002	0.003	0.007	ND	10	6	1	bd	bd	bd
2.	SHELL2	bd	0.258	3.0	1.2	4.6	bd	0.003	0.004	0.007	ND	3	2	1	bd	0.001	0.006
3.	SHELL3	bd	0.203	3.1	2.6	5.8	bd	0.002	0.003	0.005	ND	2	2	0	bd	0.001	0.015
4.	SHELL4	bd	0.140	3.1	bd	2.8	bd	0.001	0.002	0.004	ND	4	3	1	bd	bd	0.001
5.	SHELL5	bd	0.245	2.9	bd	2.9	bd	0.001	0.005	0.010	ND	8	5	1	bd	0.001	0.002
6.	SHELL6	bd	0.045	2.8	bd	2.8	4	0.001	0.001	0.002	ND	3	1	bd	bd	bd	bd
7.	SHELL7	bd	0.115	2.9	bd	2.9	bd	0.002	0.001	0.004	ND	3	3	1	bd	bd	bd
8.	SHELL8	bd	0.195	3.1	0.4	3.6	bd	0.002	0.001	0.003	ND	3	2	1	bd	0.002	0.004
9.	SHELL9	bd	0.218	3.1	bd	3.1	bd	0.011	0.006	0.022	ND	22	16	2	bd	bd	bd
10.	SHELL10	bd	0.145	3.0	bd	3.0	bd	0.001	bd	0.002	ND	9	4	1	bd	bd	0.001

ND - not determined (analyzer not functioning)
bd - below detection limit of analyzer

Table A2 **Maximum concentrations measured during the Shell Chemicals Upset.**

				Hydrocarbons				Oxides of Nitrogen				Particulates			Sulphur Compounds		
	Dataset Name	NH_3	CO	CH_4	RHC	THC	PAH	NO_2	NO	NO_x	O_3	TSP	PM_{10}	$PM_{2.5}$	H_2S	TRS	SO_2
		ppm	ppm	ppm	ppm	ppm	ng/m³	ppm	ppm	ppm	ppm	µg/m³	µg/m³	µg/m³	ppm	ppm	ppm
1.	SHELL1	0.059	0.465	2.7	0.2	2.8	55	0.018	0.152	0.152	ND	357	224	31	0.002	0.002	0.134
2.	SHELL2	bd	2.130	4.9	6.7	10.4	16	0.011	0.005	0.015	ND	42	19	3	0.001	0.003	0.023
3.	SHELL3	bd	0.310	5.7	6.3	9.0	bd	0.007	0.005	0.012	ND	58	36	4	0.001	0.003	0.024
4.	SHELL4	0.013	1.275	6.3	1.1	5.5	5	0.014	0.226	0.085	ND	152	93	7	0.001	0.000	0.011
5.	SHELL5	0.021	0.385	2.9	bd	2.9	8	0.038	0.022	0.042	ND	18	13	2	bd	0.002	0.005
6.	SHELL6	0.001	0.215	2.9	bd	2.9	4	0.003	0.003	0.003	ND	37	25	7	bd	bd	bd
7.	SHELL7	0.010	0.210	3.1	bd	3.1	5	0.014	0.006	0.020	ND	13	6	2	bd	0.001	0.001
8.	SHELL8	bd	0.250	4.3	2.1	5.3	9	0.009	0.008	0.016	ND	160	84	6	bd	0.003	0.015
9.	SHELL9	0.042	1.510	3.8	0.2	3.8	20	0.099	0.035	0.113	ND	601	398	53	bd	0.002	0.004
10.	SHELL10	0.008	1.445	3.1	0.2	3.2	9	0.007	0.046	0.046	ND	108	44	6	bd	0.002	0.017

ND - not determined (analyzer not functioning)
bd - below detection limit of analyzer

Table A1 Median concentrations measured during the Shell Chemicals Upset.

				Hydrocarbons				Oxides of Nitrogen				Particulates			Sulphur Compounds		
Dataset Name		NH_3	CO	CH_4	RHC	THC	PAH	NO_2	NO	NO_X	O_3	TSP	PM_{10}	$PM_{2.5}$	H_2S	TRS	SO_2
		ppm	ppm	ppm	ppm	ppm	ng/m^3	ppm	ppm	ppm	ppm	$\mu g/m^3$	$\mu g/m^3$	$\mu g/m^3$	ppm	ppm	ppm
1.	SHELL1	bd	0.035	2.7	bd	2.7	bd	0.002	0.003	0.007	ND	10	6	1	bd	bd	bd
2.	SHELL2	bd	0.258	3.0	1.2	4.6	bd	0.003	0.004	0.007	ND	3	2	1	bd	0.001	0.006
3.	SHELL3	bd	0.203	3.1	2.6	5.8	bd	0.002	0.003	0.005	ND	2	2	0	bd	0.001	0.015
4.	SHELL4	bd	0.140	3.1	bd	2.8	bd	0.001	0.002	0.004	ND	4	3	1	bd	bd	0.001
5.	SHELL5	bd	0.245	2.9	bd	2.9	bd	0.001	0.005	0.010	ND	8	5	1	bd	0.001	0.002
6.	SHELL6	bd	0.045	2.8	bd	2.8	4	0.001	0.001	0.002	ND	3	1	bd	bd	bd	bd
7.	SHELL7	bd	0.115	2.9	bd	2.9	bd	0.002	0.001	0.004	ND	3	3	1	bd	bd	bd
8.	SHELL8	bd	0.195	3.1	0.4	3.6	bd	0.002	0.001	0.003	ND	3	2	1	bd	0.002	0.004
9.	SHELL9	bd	0.218	3.1	bd	3.1	bd	0.011	0.006	0.022	ND	22	16	2	bd	bd	bd
10.	SHELL10	bd	0.145	3.0	bd	3.0	bd	0.001	bd	0.002	ND	9	4	1	bd	bd	0.001

ND = not determined (analyzer not functioning)
bd = below detection limit of analyzer

Table A2 Maximum concentrations measured during the Shell Chemicals Upset.

				Hydrocarbons				Oxides of Nitrogen				Particulates			Sulphur Compounds		
Dataset Name		NH_3	CO	CH_4	RHC	THC	PAH	NO_2	NO	NO_x	O_3	TSP	PM_{10}	$PM_{2.5}$	H_2S	TRS	SO_2
		ppm	ppm	ppm	ppm	ppm	ng/m³	ppm	ppm	ppm	ppm	µg/m³	µg/m³	µg/m³	ppm	ppm	ppm
1.	SHELL1	0.059	0.465	2.7	0.2	2.8	55	0.018	0.152	0.152	ND	357	224	31	0.002	0.002	0.134
2.	SHELL2	bd	2.130	4.9	6.7	10.4	16	0.011	0.005	0.015	ND	42	19	3	0.001	0.003	0.023
3.	SHELL3	bd	0.310	5.7	6.3	9.0	bd	0.007	0.005	0.012	ND	58	36	4	0.001	0.003	0.024
4.	SHELL4	0.013	1.275	6.3	1.1	5.5	5	0.014	0.226	0.085	ND	152	93	7	0.001	0.000	0.011
5.	SHELL5	0.021	0.385	2.9	bd	2.9	8	0.038	0.022	0.042	ND	18	13	2	bd	0.002	0.005
6.	SHELL6	0.001	0.215	2.9	bd	2.9	4	0.003	0.003	0.003	ND	37	25	7	bd	bd	bd
7.	SHELL7	0.010	0.210	3.1	bd	3.1	5	0.014	0.006	0.020	ND	13	6	2	bd	0.001	0.001
8.	SHELL8	bd	0.250	4.3	2.1	5.3	9	0.009	0.008	0.016	ND	160	84	6	bd	0.003	0.015
9.	SHELL9	0.042	1.510	3.8	0.2	3.8	20	0.099	0.035	0.113	ND	601	398	53	bd	0.002	0.004
10.	SHELL10	0.008	1.445	3.1	0.2	3.2	9	0.007	0.046	0.046	ND	108	44	6	bd	0.002	0.017

ND - not determined (analyzer not functioning)
bd - below detection limit of analyzer

Table A3 Weather conditions and operator remarks recorded during the Shell Chemicals Upset

Dataset Name	Time	Temp.	Relative Humidity	Wind Speed	Wind Direction	Operator Remarks
	(MST)	°C	%	km/h	degrees	
SHELL1	12:28 – 13:22	4.8	35.5	ND	ND	Slightly elevated SO_2 no RHC detected.
SHELL2	13:27 – 14:26	4.0	31.1	37.3	314	Epoxy-like odours.
SHELL3	14:27 – 15:26	4.1	32.1	31.8	313	Epoxy-like odours.
SHELL4	15:27 – 16:11	4.7	32.6	20.3	298	Few elevated concentrations.
SHELL5	16:12 – 16:32	3.5	35.3	32.3	65	No elevated concentrations.
SHELL6	16:34 – 16:45	3.8	34.5	ND	ND	No elevated concentrations.
SHELL7	16:46 – 17:01	3.9	32.0	36.0	322	Detect odours.
SHELL8	17:02 – 17:54	3.2	32.0	24.0	297	Very few elevated concentrations.
SHELL9	17:56 – 18:11	2.2	32.0	ND	ND	No elevated concentrations.
SHELL10	18:11 – 19:24	0.3	36.6	11.2	127	No elevated concentrations.

ND – not determined (The MAML cannot determine wind direction or speed while mobile)

Table A3 **Weather conditions and operator remarks recorded during the Shell Chemicals Upset**

Dataset Name	Time (MST)	Temp. °C	Relative Humidity %	Wind Speed km/h	Wind Direction degrees	Operator Remarks
SHELL1	12:28 – 13:22	4.8	35.5	ND	ND	Slightly elevated SO_2, no RHC detected.
SHELL2	13:27 – 14:26	4.0	31.1	37.3	314	Epoxy-like odours.
SHELL3	14:27 – 15:26	4.1	32.1	31.8	313	Epoxy-like odours.
SHELL4	15:27 – 16:11	4.7	32.6	20.3	298	Few elevated concentrations.
SHELL5	16:12 – 16:32	3.5	35.3	32.3	65	No elevated concentrations.
SHELL6	16:34 – 16:45	3.8	34.5	ND	ND	No elevated concentrations.
SHELL7	16:46 – 17:01	3.9	32.0	36.0	322	Detect odours.
SHELL8	17:02 – 17:54	3.2	32.0	24.0	297	Very few elevated concentrations.
SHELL9	17:56 – 18:11	2.2	32.0	ND	ND	No elevated concentrations.
SHELL10	18:11 – 19:24	0.3	36.6	11.2	127	No elevated concentrations.

ND – not determined (The MAML cannot determine wind direction or speed while mobile)